Journal of Statistical Physics, Vol. 30, No. 2, 1983

Stochastic Processes Originating in Deterministic Microscopic Dynamics

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We investigate the probability distribution of the scaled trajectory of a test particle moving in an equilibrium fluid according to the laws of classical mechanics, i.e., if $Q(t)$ is the displacement of the test particle we let $Q_A(t) = Q(At)/\sqrt{A}$ and consider the distribution of the trajectory $Q_A(t)$ in the limit $A \to \infty$. The randomness of the motion is due entirely to the randomness of the initial state of the fluid, test particle, or both, and the process is generally non-Markovian. Nevertheless, it can be proven in some cases and we expect it to be true in many more that $Q_A(t)$ looks like Brownian motion in the limit $A \to \infty$. Some results for simple model systems are presented.

KEY WORDS: Central limit theorem; Brownian motion; test particle; deterministic dynamics; stochastic processes; invariance principle.

1. INTRODUCTION

This article is based on our work in progress concerning the motion of a test particle in an infinite classical mechanical system of particles, when this motion is viewed on macroscopic time and length scales. The test particle can, but need not, be mechanically identical to the other particles (the *fluid particles*) of the system. When it is identical we single it out by its different "color." In either case we expect that on the macroscopic scale many details will become unimportant and the motion of the test particle will have a universal form, i.e., Brownian motion.

Presented at the Symposium on Random Walks, Gaithersburg, MD, June 1982.

* Supported in part by NSF Grants DMR 81-14726 and PHY 78-03816.

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The mathematical formulation of our problem is as follows: Let Q, V denote the position and velocity of the test particle and (q_i, v_i) $i = 1, 2, \ldots,$ the positions and velocities of the fluid particles. We assume that at time $t = 0$ the microscopic state of the system, given by $(Q, V, q_1, v_1, \ldots)$, is distributed according to the appropriate conditional Gibbs distribution with the initial position Q_0 of the test particle given, say $Q_0 = 0$, i.e., apart from the position of the test particle the system is in thermodynamic equilibrium. We now observe the motion of the test particle, i.e., its position $Q(t)$ and its velocity $V(t)$ as functions of time t. $Q(t)$ and $V(t)$ define stochastic processes on the probability space of microscopic states, for which the average will be denoted by $E(\ )$. Note that $E(V(t)) = 0$.

Since we wish to describe the motion of the test particle on a macroscopic scale we introduce the process

$$Q_A(t) = Q(At)/\sqrt{A}$$

and consider the limit $A \to \infty$. We have that

$$Q_A(t) = A^{-1/2} \int_0^{At} V(s)\, ds$$

or setting $A = N$, an integer,

$$Q_N(t) = N^{-1/2} \sum_{j=0}^{N-1} \left[\int_{jt}^{(j+1)t} V(s)\, ds \right] = N^{-1/2} \sum_{j=0}^{N-1} X_j$$

so that if the increments

$$X_j = \int_{jt}^{(j+1)t} V(s)\, ds, \qquad j = 0, \ldots, N-1$$

were independent, it would follow from the central limit theorem (CLT) that $Q_N(t)$ converges in distribution to a Gaussian random variable as $N \to \infty$. Moreover, it would follow from Donsker's invariance principle[1] that the process $Q_A(t)$ converges in distribution to the Brownian motion $W_D(t)$, $Q_A \to W_D$, where $D = 2\int_0^\infty E(V(0) \cdot V(t))\, dt$ and $E(W_D^2(t)) = Dt$. $Q_A \to W_D$ means that for any "continuous" function f on the space of trajectories $Q(t)$, $0 \leqslant t < \infty$, $E(f(Q_A)) \to E(f(W_D))$ as $A \to \infty$. This implies, in addition to the convergence of all finite-dimensional distributions for Q_A, i.e., the joint distributions of $Q_A(t_1), \ldots, Q_A(t_n)$, $t_1 < \cdots < t_n$, to the corresponding distributions for W_D, the convergence of such quantities as the maximum of $Q(t)$, $0 \leqslant t \leqslant T$. In fact, $Q_A \to W_D$ implies that if one does not observe the motion on too fine a scale, the process Q_A cannot be distinguished from the Brownian motion W_D for A sufficiently large.

In an infinite classical system the increments X_j will not be independent, in part because X_j will be correlated with the velocity of the test particle at the end of the jth time interval, which will affect the increment X_{j+1} in the next interval, and in part because some of the interactions experienced by the test particle in different time intervals will involve the same or correlated fluid particles. For example, even in the very simple case of a spherical test particle undergoing elastic collisions with an (otherwise) ideal gas of point particles, the test particle may recollide, perhaps after a very long time, with the same fluid particle. Thus from the past trajectory of the test particle we may extract information about its future evolution. It follows that, far from having independent position increments, the process $(Q(t), V(t))$ will not be Markovian.

However, since the increment in position over a macroscopic time interval is the effect of a large number of interactions, most of which involve only fresh fluid particles which were not involved directly in interactions with the test particle prior to this interval, we expect that $Q_A(t)$ can be decomposed into a sum of increments which are approximately independent and that $Q_A \to W_D$. We also expect that generally we will have $D > 0$. If $Q_A \to W_D$ with $D > 0$, we say that the system (or the test particle) has *diffusive behavior*. [Since $W_0(t) = 0$ the convergence $Q_A(t) \to W_0$ does not well express diffusive behavior.]

The formula

$$D = 2\int_0^\infty E(V(0) \cdot V(t))\, dt \tag{1}$$

for the diffusion coefficient is suggested by the observation that if the velocity autocorrelation function

$$R(t) = E(V(0) \cdot V(t))$$

is integrable, then

$$\lim_{t\to\infty} t^{-1} E\big(Q(t)^2\big) = D$$

where D is given by (1). If the past and future in the velocity process $V(t)$ are sufficiently independent, $R(t)$ will be integrable and D will be well defined and finite, $D < \infty$.

The integrability of the velocity autocorrelation function may be regarded as a minimal condition for $Q_A \to W_D$. It is, however, not sufficient because (i) it does not guarantee sufficient independence for a CLT, and (ii) no matter how strong the independence properties, nothing precludes the possibility that $D = 0$. [Consider, for example, a particle undergoing an Ornstein Uhlenbeck process in a harmonic potential:

$$dQ = V\,dt$$

$$dV = (-\gamma Q - \delta V)\,dt + \sigma\, dW_1$$

The Markov process $(Q(t), V(t))$ has very strong independence of past and future; the distribution of $Q(t), V(t)$ converges to equilibrium exponentially fast. Nonetheless $D = 0$, precisely because of the existence of a (normalizable) equilibrium distribution to which $(Q(t), V(t))$ converges in distribution.]

We remark that though the integrability of the velocity autocorrelation function does not in general guarantee diffusive behavior, there is one case in which it does, namely, when the velocity is a function of the state of a reversible Markov process.[2,3] However, this cannot be the case for a purely mechanical system.

2. SOME RESULTS

From a physical point of view, the most interesting of the models for which we would like to establish diffusive behavior is the three-dimensional system of interacting particles, e.g., the *hard sphere gas*, where the infinitely extended fluid consists of identical hard spheres which interact via elastic collisions. The test particle may be a colored fluid-sphere or it may be a dynamically distinguishable sphere having, say, a different mass or radius. A simplified version of the latter case is the system already mentioned in which the fluid consists of point particles, so that fluid particles do not interact with each other, i.e., a *hard sphere in an ideal gas*. In one dimension the models described reduce to the case of a hard point system where the fluid can always be taken to be an ideal gas. If the mass of the test particle in this system of particles moving on a line is the same as that of the fluid particles we have the *equal mass* case; otherwise, we have the *unequal mass case*.

Harris and Spitzer[4,5] (see also Jepsen[6] and Lebowitz and Percus[7]) have established diffusive behavior for the equal mass case. Their argument is very special, and does not extend to the unequal mass case, let alone to higher dimensions. It exploits the fact that in the equal mass case the motion of the test particle may be obtained by keeping track of the "pulse," in an ideal gas of completely noninteracting "pulses," on which the test particle is riding: when pulses cross, the test particle changes its horse. This description allows them to express the distribution of $Q(t)$ in terms of the easily computable probabilities of certain "elementary" events.

Sinai and Bunimovich[8,9] have established diffusive behavior for the two-dimensional periodic Lorentz gas. Here the test particle is a point particle moving with unit speed among a periodic array of convex scatters so arranged that the time between collisions is bounded away from zero and infinity. The only randomness lies in the initial distribution of the position and direction of motion of the test particle, which is assumed to be given by a smooth density. [If this distribution is uniform over a fundamental domain, the velocity process $V(t)$ is stationary.] Their proof exploits the existence of a "Markov partition," which provides a representation in terms of a symbolic dynamics in which past and future are asymptotically independent.

These two models are essentially the only completely mechanical ones for which diffusive behavior has been established. In particular, diffusive behavior has not been established, though it is certainly expected, for the unequal mass case in one dimension, for a sphere in an ideal gas (in two or more dimensions), for the hard sphere gas in three or more dimensions, and for the Lorentz gas with random scatterers in two or more dimensions. The fact that diffusive behavior is not even expected for the hard sphere gas in two dimensions is connected with the phenomenon of long time tails in the velocity autocorrelation function: Computer simulations and physical arguments indicate that $D = \infty$ in this case.[10]

3. METHODS AND MODELS

Establishing diffusive behavior is referred to in the mathematical literature as proving a functional CLT or an invariance principle. The basic results provide conditions under which a stationary process $V(t)$ with $E(V(t)) = 0$, not necessarily arising from a mechanical system, leads to diffusive behavior: $Q_A \to W_D$, where $Q_A(t) = A^{-1/2}\int_0^{At} V(s)\,ds$. These conditions always involve, in many inequivalent forms, an expression of asymptotic independence of past and future for the process $V(t)$. Some of them are referred to as *mixing conditions*, of which there are many, of varying strengths, all of which are stronger than the familiar notion of mixing used in ergodic theory; the process $V(t)$ is mixing in the ergodic theoretic sense if

$$E(fg_\tau) - E(f)E(g) \underset{\tau\to\infty}{\to} 0 \tag{2}$$

where f and g are square-integrable functions of $\{V(t)\}_{t\in R} \equiv V(\cdot)$ and $g_\tau(V(\cdot)) = g(V(\tau + \cdot))$. For example, $V(t)$ is called α-*mixing* (strongly mixing, Rosenblatt mixing) if $\sup[E(fg) - E(f)E(g)] \equiv \alpha(\tau) \to 0$, as $\tau \to \infty$, where the sup is over all (measurable) functions $f, |f| \leqslant 1$, depending only upon the past of the velocity process [i.e., on $V(t)$ for $t \leqslant 0$] and g, $|g| \leqslant 1$, depending only upon the future after time τ [$V(t)$, $t \geqslant \tau$].

It can be shown[11] that $\alpha(\tau)$ provides an upper bound for the velocity autocorrelation function: If $V(t)$ has $n > 2$ moments, $E(|V(t)|^n) < \infty$, then

$$E(V(0) \cdot V(\tau)) \leqslant \text{const}\, \alpha(\tau)^{1-2/n} \tag{3}$$

Moreover if $V(t)$ is α-mixing with

$$\int_0^\infty \alpha(t)^{1-2/n}\,dt < \infty \tag{4}$$

then $Q_A \to W_D$. If (4) is satisfied we say that the process $V(t)$ is *rapidly α-mixing*. Diffusive behavior follows from rapid α-mixing once $D > 0$ has also been established.

We remark again that the question of whether $D > 0$ is frequently nontrivial. A simple condition guaranteeing $D > 0$ is described at the end of this paper.

Rapid α-mixing is generally difficult to establish; in fact, it is usually quite difficult to obtain merely a good estimate of the velocity autocorrelation function. However, in case the velocity is a function of the state of an ergodic, mixing Harris process[12,13] we can begin to get a handle on $\alpha(\tau)$. A Markov process $X(t)$, with transition probability π_x^τ [$\pi_x^\tau(A)$ is the probability that $X(\tau) \in A$ given that $X(0) = x$] and stationary distribution π [$\int \pi(dx)\pi_x^\tau(\cdot) = \pi(\cdot)$] is a *Harris process* if π_x^τ overlaps (i.e., is not mutually singular with respect to) π for τ sufficiently large. If the process also has no nontrivial invariant sets, we have a *mixing Harris process* and

$$\|\pi_x^\tau - \pi\| \equiv \sup_{|f(x)| \leqslant 1} \left[\pi_x^\tau(f) - \pi(f)\right] \xrightarrow[\tau\to\infty]{} 0$$

Now suppose the velocity $V(t) = V(X(t))$ is a function of the state at time t of a mixing Harris process. Then, using the Markov property, it is easy to see that $\alpha(\tau) \leqslant \int \pi(dx)\,\|\pi_x^\tau - \pi\|$, so that $V(t)$ is α-mixing. Moreover, if we have some fairly weak control over the "overlap" of π_x^τ and $\pi_{x'}^\tau$ in the transition probabilities as we vary τ and the starting points x and x' —in which case we say that $X(t)$ is *a good* mixing Harris process—the decay of $\|\pi_x^\tau - \pi\|$ will be sufficiently fast that $V(t)$ is rapidly α-mixing.[13]

We now describe a couple of "one-dimensional" mechanical models for which we believe diffusive behavior can be established by representing the velocity process as a function of the state of a good mixing Harris process.[13]

(i) The test particle is a vertical line segment (stick) of length 1 centered on the x axis. This stick, which cannot rotate and can move only horizontally, interacts with a two-dimensional ideal gas of fluid particles, undergoing elastic collisions which do not alter the y component v_y of the fluid particle velocities. The velocity process will be stationary if the distribution of the x component of the fluid particle velocities is Maxwellian, for any distribution of v_y. Since the stick cannot recollide with a fluid particle once it leaves the strip S of length 1 centered around the x axis, we obtain a stationary Markov process by observing only the particles inside S, keeping track of positions only relative to the stick. Suppose now that for all fluid particles $|v_y| > a > 0$. Then this process should be a good mixing Harris process, since all fluid particles in S at $t = 0$ will have been replaced by fresh particles by time $t = 1/a$.

(ii) Suppose now that the stick (of length 1) is centered on, and perpendicular to, the circle of radius 1 centered at the origin. Suppose again that the stick interacts via elastic collisions with a two-dimensional ideal gas, whose particles are also elastically reflected from a circular wall of radius 1/2 centered at the origin. Now V represents the (angular) velocity of the stick around the "race track," so that $Q(t)$ is the angle $\theta(t)$ attained by time t, where $\theta(t)$, $t \geqslant 0$, $-\infty < \theta < \infty$, is continuous. We obtain a stationary Markov process, which again should be a good mixing Harris process, by observing only particles in the annulus S of inner radius 1/2 and outer radius 3/2. Though it is now possible for fluid particles to remain in S for an arbitrarily long time, we can guarantee their departure by sending into S appropriate fluid particles.

In the models of primary interest rapid α-mixing is probably too much to demand. Consider first the equal mass case in one dimension. Jepsen[6] has shown that $E(V(0) \cdot V(t)) \sim t^{-3}$. Since the velocity distribution is Maxwellian, $V(t)$ has moments of all orders; it thus follows from (3) that $\alpha(\tau) \geqslant \text{const}\, t^{-(3+\epsilon)}$, $\epsilon < 0$, which suggests that establishing (4) may, at best, be quite delicate. In fact, estimates involving slow fluid particles suggest that $\alpha(\tau)$ is bounded away from zero, so that $V(t)$ is not even α-mixing, and this is true even in the unequal mass case, where we expect a much faster (perhaps exponential) decay of the velocity autocorrelation function.

There are conditions for diffusive behavior, weaker than rapid α-mixing, which do not require that the entire future of the velocity process be asymptotically independent of the past, nor even that this be true of the velocity $V(t)$ at a single large time t. For example, suppose $V(t)$ is a stationary ergodic process with $n \geqslant 2$ moments, and let $p = n/(n-1)$. If the conditional expectation $\hat{V}(\tau)$ of $V(\tau)$ given the past $[V(t),\ t \leqslant 0]$ satisfies

$$\int_0^\infty \|\hat{V}(t)\|_p \, dt < \infty \tag{5}$$

then $Q_A \to W_D$. Here $\|\hat{V}(t)\|_p = [E(|\hat{V}(t)|^p)]^{1/p}$. Moreover, if $\|Q(t)\|_p$ is unbounded (as $t \to \infty$) then $D > 0$ and we have diffusive behavior. This result is based on a circle of ideas revolving around the martingale difference CLT.[1,2]

It appears likely that (5) is satisfied in all the models discussed here, though proving that this is so is probably quite difficult. Note that since

$\| \hat{V}(\tau) \|_p \leqslant \text{const}\, \alpha(\tau)^{(n-2)/2}$, the condition (5) is weaker than rapid α-mixing. Nonetheless, unless the velocity is a function of the state of a reversible Markov process, so that the self-adjointness of the generator can be exploited, $\| \hat{V}(\tau) \|_p$ is difficult to estimate without employing Markovian methods which provide a good estimate for $\alpha(\tau)$. For example, this is the case in the models (i) and (ii) in which the velocity is a function of the state of a good mixing Harris process.

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